



Max-Born-Institut

## Masterarbeit



### Computing Band Alignments in Group-IV Optoelectronic Structures

#### Project Description

One of the concepts for further increasing the performance of integrated circuits is to equip them with optical communication channels. While Si is notoriously bad at emitting light, alloys of SiGeSn are CMOS-compatible and have recently been shown to exhibit a direct bandgap for certain compositional ranges. This suggests to develop optoelectronic devices based SiGeSn-based heterostructures, such as quantum wells and quantum dots.

Consequently, it is imperative to determine the band alignment near the interfaces between different materials as this provides the potential landscape in which electrons and holes move and, therefore, strongly influences optical transition energies etc. Density functional theory (DFT) provides an ideal framework for modeling such band alignments and, specifically, the focus of this master thesis will be on the computations of the band alignment between the elementary semiconductors Si, Ge, and Sn via DFT. This work is important and timely as the theoretical investigations published so far are contradictory and corresponding experimental studies on interfaces are extremely challenging.

Within this master thesis, you have the opportunity to learn more about:

- Group-IV optoelectronic device technology
- Numerical band structure techniques (with focus on DFT)
- Theory of semiconductor interfaces
- How to have fun doing atomistic material modeling.

Furthermore, the results of your work will be directly used by our experimental collaborators at University of Stuttgart for their experimental designs.

#### Prerequisites

Good knowledge in solid state physics/semiconductor physics and optics. Enjoying working with computers and interest in computational physics; Programming skills are helpful but not required.

#### Contact

If you are interested, please contact M.Sc. Torsten Wendav ([wendav@physik.hu-berlin.de](mailto:wendav@physik.hu-berlin.de), Tel. 7618) or Prof. Dr. Kurt Busch ([kbusch@physik.hu-berlin.de](mailto:kbusch@physik.hu-berlin.de))